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Neural network representation for electron and positron collisions with sodium and potassium atoms

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Abstract : An artificial neural network (ANN) has been designed to simulate the collisions of electrons and positrons with sodium and potassium atoms at low and intermediate energies. The ANN model has been trained based on experimental data to produce the total cross sections for each case. Levenberg-Marquardt algorithm (LMA) has been employed to train the ANN. The experimental, trained and calculated total collisional cross sections are compared. The designed ANN shows a good match to the experimental data.

Keywords : Neural network, electron and positron collisions, sodium and potassium atoms, total collisional cross sections.

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1. Introduction

Alkali-metal atoms have been a subject of interest in several recent theoretical and experimental investigations in electron (positron)-atom scattering because of their various interesting properties : relatively simple structure, low ionization potentials (3.9–5.4 eV) and existence of resonance lines in the visible or quartz ultraviolet part of the electromagnetic spectrum.

The total scattering cross sections have been measured [1] or estimated (see for example Refs. [2–8] and references therein) by various groups using different approximations. Most of the approximations take into account either the atomic distortion (through excited states and polarization) or the rearrangement process (positron (Ps) formation in case of positron scattering) or both.

In the collisions of positrons and electrons with atoms, two interactions play important role. The static interaction (associated with the interaction of the projectile with the Coulomb field of the undistorted atom) is attractive for the electron and repulsive for the positron, while the polarization interaction (resulting from the distortion of the atom by the charged projectile) is attractive for both projectiles. The net effect of the static and polarization interactions is that they add to each other in electron scattering whereas they tend to cancel each other in positron scattering. In general, this results in smaller total scattering cross sections for positrons than for electrons at low energies. As the projectile energy is increased, the polarization and exchange interactions (the exchange interaction contributes to electron scattering due to the indistinguishability of the projectile and electrons in the target atom but does not play a role in positron scattering) eventually become negligible compared with the static interaction, and the expected result is a merging of the corresponding positron and electron scattering cross sections at sufficiently high projectile energies. Therefore, at low energies the target atom is distorted by the projectile and the dominant interaction is the polarization interaction. At high energies, the overall interaction is dominant by the static Coulomb field of the target atom.

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The experimental results show that unlike for other target atoms, the total scattering cross sections for the alkali atoms are slightly larger at low energies for positrons than for electrons, most probably because of a significant positronium formation component in the case of the former projectile.

Recently, artificial neural network (ANN) has been one of researchers, interests in modelling of high energy physics [9]. In the present work, we have developed an artificial neural network, as a first treatment, to describe the scattering of electrons and positrons by sodium and potassium atoms. Neural networks are fed with some parameters describing the required interaction and then trained so that the outputs imitate the experimental data. Section 2 of this paper presents the summary of our theoretical treatment of the coupled-static frozen-core approximation. Section 3 deals with the development of the proposed neural network. Finally, in Section 4, we present our results and conclusion.

2. Coupled-static frozen-core treatment

The study of any atomic scattering problems requires the solution of the Schrödinger equation

$$(H-E)|\Psi\rangle=|0\rangle, \tag{1}$$

where H and Ψ are the **exact** total Hamiltonian and total wavefunction, respectively, corresponding to a given total energy E. Although, in most atomic processes H and E are known, the evaluation of $|\Psi\rangle$ is subjected to various methods of approximation. The first step in all these methods is Born-Oppenheimer's adiabatic approximation in which it is assumed that the nucleus of the target is infinitely heavy and thus is regarded to be fixed at the origin of the configuration space. For the collision of light particles with atoms, further assumptions are made such as frozen-core or fixed-core approximation, *i.e.* the alkali atoms are treated as one-electron atoms. In other words, the valence electron of any alkali atom is considered as to move in a fixed effective potential. The inelastic collisions under consideration can be sketched by

e^+ + A (ground)
- $\rightarrow$ e^+ + A (ground), (elastic channel);
- $\rightarrow$ Ps (ground), + A^+, (ground Ps channel);
- $\rightarrow$ Ps* (excited), + A^{+*}, (excited Ps formation channel);
- $\rightarrow$ $e^{+'}$ +A* (excited), (excitation channel);
- $\overline{\downarrow\rightarrow}$, ($n$-th channel).

In the coupled-static approximation, the total wavefunction Ψ is expressed by

$$|\Psi\rangle=|\Psi_1\rangle+|\Psi_2\rangle+|\Psi_3\rangle+...+|\Psi_n\rangle$$

$$=|\phi_1\rangle|\psi_1\rangle+|\phi_2\rangle|\psi_2\rangle+|\phi_3\rangle|\psi_3\rangle+...+|\phi_n\rangle|\psi_n\rangle, \tag{2}$$

where ϕ_i's and ψ_i's (i = 1, 2, 3...n) are the bound state and the scattering wavefunctions, respectively, of the considered channels. n refer to the channel number and at the same time equals the number of channels under consideration. The coupled-static approximation demands that

$$\langle\phi_i|H-E|\Psi\rangle=0, \ (i = 1, 2, 3...n). \tag{3}$$

The total energy $E = E^{(i)}$ (the total energy of the channel i, *i.e.* $E = E^{(1)} = E^{(2)} = ... = E^{(n)}$). The frozen-core model of the channel is described by the total Hamiltonian $H = H^{(i)}$ (the total Hamiltonian of the channel i, *i.e.* $H = H(1) = H^{(2)} = ...= H^{(n)}$ such that

$$H^{(i)} = H_T^q - \nabla_x^2 + V_{\text{int}}^{q(i)}. \tag{4}$$

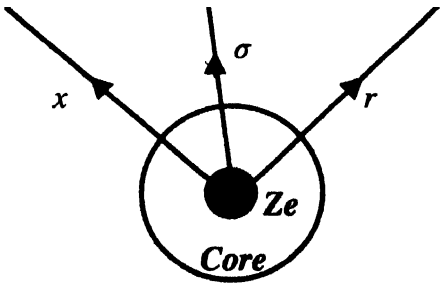

Figure 1. Configuration space of positron-alkali atom scattering.

The one-valence electron model of an alkali target q is described (in Rydberg units) by the Hamiltonian

$$H_T^q=-\nabla_r^2-\frac{2}{r}+V_C^q(r), \tag{5}$$

where the potential $(-2/r)$ represents the Coulomb interaction between the valance electron of position vector r and the screened nuclear charge ($=Z^q e - N^q e$; Z^q and N^q are the atomic number and the number of core electrons, respectively, of the target q). $V_C^q(r)$ is a screened core potential and $V_{\text{int}}^{q(i)}$ is the interaction potential of the channel i (see *e.g.* Refs. [6,8] and [10–12]).

The iterative Green-function partial-wave expansion technique described in details in Refs. [11] and [8] within the framework of the coupled-static approximation (CSA3C) is employed in order to calculate the reactance

and transition matrices (R and T, respectively) required for the evaluation of the partial and total cross sections of the first, second and third channels (*i.e.* n = 3). The partial cross sections corresponding to the total angular momentum ℓ are determined (in πa_0^2 units) after the v-th iteration as

$$\sigma_{ij}^{(\ell,v)}=\frac{4(2\ell+1)}{k_i^2}\left|T_{ij}^{v}\right|^2, \quad i,j=1,2,\ldots,n \tag{6}$$

where T_{ij}^{v} is the iterative transition matrix element. The total cross sections are given (in πa_0^2 units) after the v-th iteration as

$$\sigma_{ij}^{v}=\sum_{\ell=0}^{\infty}\sigma^{(\ell,v)} \quad i,j=1,2,\ldots,n \tag{7}$$

3. Neural network representation for the scattering of electrons and positrons by Na and K atoms

3.1. Feedforward neural networks :

An artificial neural network (ANN) is made up of a number of simple and highly inter-connected computational elements. There are many types of ANNs, but all of them have three things in common : individual neurons (processing elements), connections (topology) and a learning algorithm. The processing element calculates the neuron transfer function of the summation of weighted inputs. A simple neuron structure is shown in the Figure

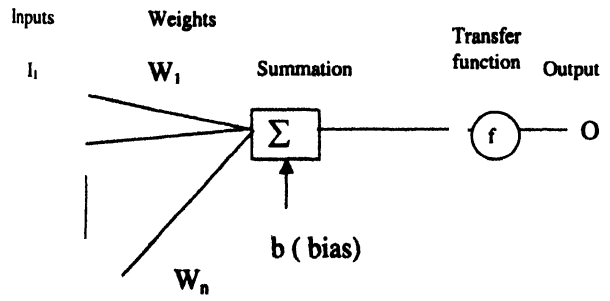

Figure 2. Neuron model.

The neuron transfer function f is typically step or sigmoid function that produces a scalar output (O) as follows

$$O=f\left(\sum_i W_i I_i + b\right) \tag{8}$$

where I_i, W_i and b are the i-th input, i-th weight and the bias, respectively.

The objective is to associate a P-pattern input to their corresponding P-pattern target. The following definitions [13–15] are necessary.

NI, NH and NO = the number of nodes in the input, hidden and output layers, respectively,

I (i, r) = the i-th input value, $i\in$(1,NI); in the r-th input pattern, r$\in$(1,P),

$W1(i,j)$ = the weight connecting the i-th input value to the j-th hidden neuron,

$B1(j)$, $j\in(1,NH)$ = the bias associated with the j-th hidden neuron,

$H(j,r)$ = the output of the j-th hidden neuron, $j\in$(1,NH), for the r-th input pattern,

$W2(j,k)$ = the weight connecting the j-th hidden neuron to the k-th output neuron,

$B2(k)$, $k\in$(1,NO) = the bias associated with the k-th output neuron,

$O(k,r)$ = output of the k-th output neuron, $k\in$(1,NO), for the r-th input pattern,

$T(k,r)$ = target of the k-th output neuron, $k\in$(1,NO), for the r-th input pattern,

Y = all weights and biases for the whole NN.

The output of the j-th hidden neuron at the r-th input pattern is given by :

$$H(j,r)=f\left[\sum_{i=1}^{NI} W1(i,j)I(i,r)+B1(j)\right] \tag{9}$$

where f is an approximate transfer function. Typical transfer functions are, the hyberbolic tangent function defined as :

$$f_1(\theta) = \tanh(\theta), \tag{10}$$

and the linear function defined as :

$$f_2(\theta) = (\theta). \tag{11}$$

Similarly, the output of the k-th output neuron is given by :

$$O(k,r)=f\left[\sum_{j=1}^{NH} W2(j,k)H(j,r) + B2(k)\right] \tag{12}$$

The NN output O, is required to mimic a target output T. To achieve that, the NN is trained to find an approximate set of weights and biases Y, which minimizes an index E

defined as :

$$E=\sum_{k=1}^{NO}\sum_{r=1}^{P}[O(k,r)-T(k,r)]^2 \quad (13)$$

An algorithm is employed to minimize the index E over Y, employing gradients estimated using the partial derivatives of E with respect to Y. The gradients are determined, employing the backpropagation technique which involves performing computations backward in the network [16]. The training is performed employing the Levenberg-Marquardt algorithm (LMA) [17]. The LMA employs a Newton-like update in the form :

$$Y_v=Y_{v-1}-\left[J^tJ-\mu\tilde{I}\right]^{-1}J^te, \quad (14)$$

where J is the Jacobian matrix which contains the first derivatives of the NN errors with respect to the weights and biases. e is a vector of NN errors, μ is a scalar changed adaptively by the algorithm (the adaptation constant), v is the iteration number, t denotes transposition and $\tilde{I}$ is the identity matrix. The term between brackets in the R.H.S. of eq. (14) is an approximation of the Hessian matrix, while the term after it, is the gradient.

3.2. The proposed neural network :

Artificial Neural Networks (ANN) are vital tools for system modelling and classification. Readers can refer to Haykin [13] for basics of ANNs structure and training methodologies.

The authors propose an ANN to model the total collisional cross section of positrons and electrons with sodium and potassium atoms at different incident energies.

The proposed network consists of input layer, one hidden layer and an output layer. The input layer composes of two inputs (Ni = 2), the first is the projectile type and the second is the incident energy.

Five neurons (Nh = 5) based on tanh activation function in the only hidden layer were found to be enough to model the collision problems of interest. The output layer uses single neuron ($N0$ = 1) based on a linear activation function. Figure 3 shows the structure of the proposed network.

The training data set of the proposed network is based on experimental data for the total scattering cross sections of the collisions of positrons and electrons with Na and K atoms [1]. The training data for Na atoms were composed of 16 input-output pairs (P = 16) for both positron and electron projectiles. Same number input-output pairs were used in case of K-atoms.

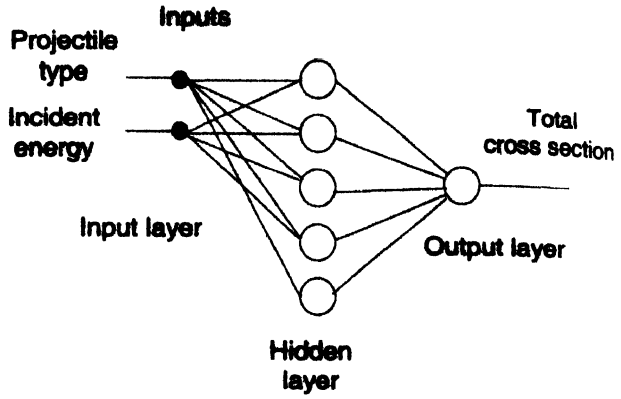

Figure 3. Proposed neural network configuration.

The initial training weights were also chosen using the Nguyen-Widrow random generator [17] in order to speed up the training process.

The network was trained twice; once for Na and another for K. The proposed ANN has been trained to associate the input patterns to the target output patterns using the Levenberg-Marquardt approximation (LMA). The final weights and biases for both networks are given in appendix.

4. Results and conclusion

The trained network was tested using the experimental data. The training data is based on experimental observations at incident energies ranging from 4.1 eV to 67.1 eV for e-Na scattering, from 4.4 eV to 101.9 eV for e-K scattering and for positron scattering by Na and K atoms the ranges are (17.7 eV to 98.3 eV) and (7.9 eV to 98.5 eV), respectively.

The mathematical formalism of the coupled-static frozen-core treatment of Section 2 has been applied to the collisions of positrons with sodium atoms taking into consideration three channels only *i.e.* n = 3. These channels are the elastic, ground positronium formation and excited positronium formation [10]. The corresponding total collisional cross sections are refered to as CSA3C. The coupled-channel-optical (CCO) method with both the equivalent-local (ELP) [18] and partial-wave (PWP) [19] calculations of the polarization potential have been also used for the comparison with our present ANN calculations. The experimental (EXP), trained (ANN) and calculated total scattering cross sections of different authors for the collisions of electrons and positrons with sodium and potassium atoms are demonstrated in Figures 4–7.

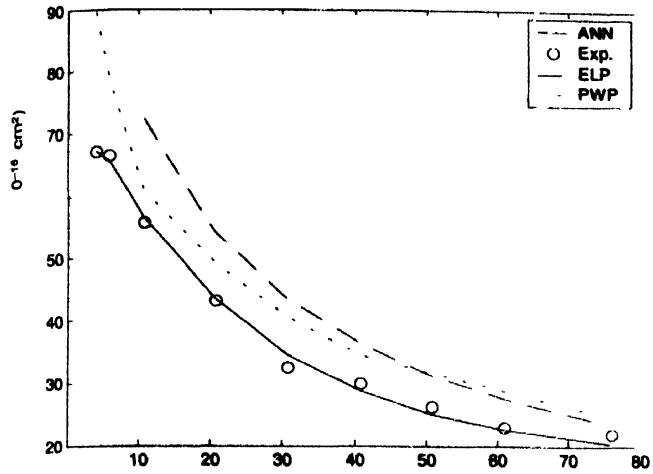

Figure 4. Total cross sections (10^{-16} cm^2) for electron-sodium scattering. ANN-present calculations using artificial neural network; Exp-experimental data [1]; ELP-theoretical calculations using coupled-channel-optical method with the equivalent-local polarization potential [18]; PWP-calculations using partial-wave polarization potential [19].

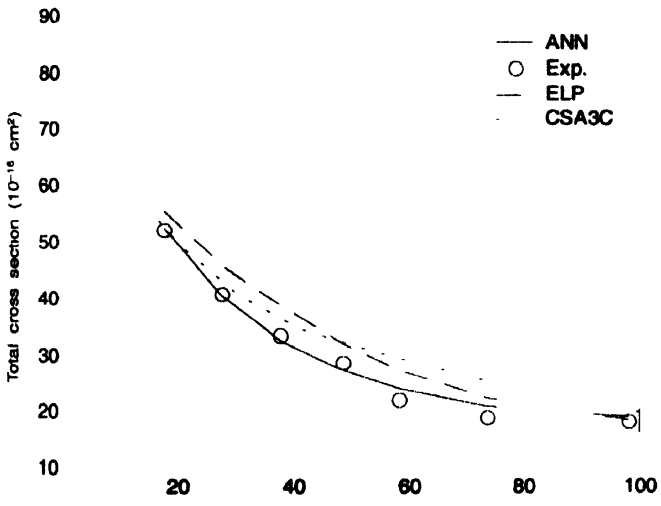

Figure 5. Same as in Figure 4, but for positron-sodium scattering. CSA3C-calculations using coupled-static approximation with three channels [10].

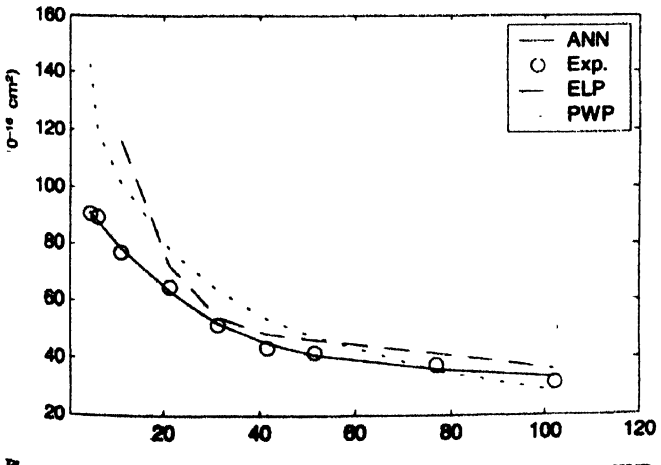

Figure 6. Same as in Figure 4, but for electron-potassium scattering. PWP-partial-wave polarization potential [20].

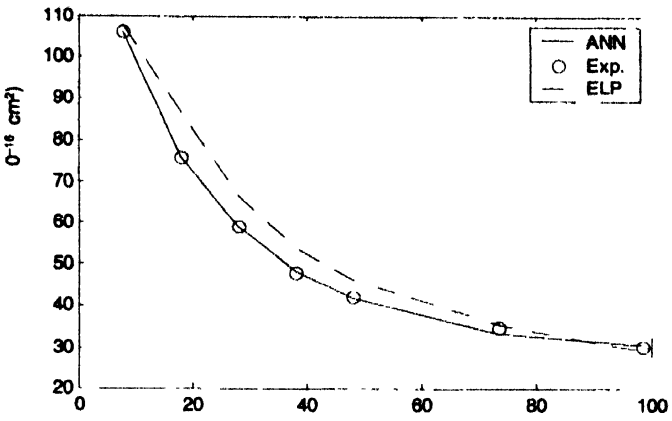

Figure 7. Same as in Figure 4, but for positron-potassium scattering.

Figures 4 and 5 show that the ELP calculation of the polarization potential gives larger cross sections than experimental for electrons at the lower energies. It is considered to be unrealistic below 10 eV, where the plane-wave and equivalent-local approximations are invalid. The PWP calculations is much better at the lower energies and usually gives a cross section within the experimental error, while tending again to overestimate. For electrons, both ELP and PWP again tend to overestimate the total cross section at energies below 10 eV, but both agree quite well at higher energies. For positrons ELP again agrees within experimental error.

Figure 6 demonstrates the importance of the inclusion of the positronium formation in the very low-energy region and shows also that our CSA3C calculations of the total cross sections [10] are more better than the corresponding ELP up to nearly 50 eV beyond which the effect of positronium formation becomes negligible.

Figures 4–7 display a good match between the experimental data and our proposed ANN. These figures show a better performance of the ANN over the other approaches.

Finally, we conclude that neural networks have become one of important research areas in the field of theoretical atomic collision physics. The present work presents a new technique for modelling the total collisional cross sections of electrons and positrons with sodium and potassium alkali atoms based on ANN approach. The designed ANN shows a good match to the experimental data and a better performance over other theoretical calculations.

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Appendix

$$W1 = \begin{pmatrix} -0.6869 & -959.5853 \\ 1.4858 & 33.9652 \\ -1.4194 & -171.3486 \\ -1.2020 & -32.3416 \\ 0.0870 & -0.0211 \end{pmatrix}$$

$B1$ = 1.0e + 003* [3.9277 0.0030 0.0449 −0.005(−0.0058]^T,

$W2$ = 1.0e + 006* [−0.6402 0.6468 −0.6469 3.2347]

$B2$ = 6.4684e + 005

Potassium Network's weights

$$W1 = \begin{pmatrix} 11.3903 & -0.1361 \\ -3.4632 & -0.0215 \\ 120.3337 & -29.9583 \\ 62.8031 & 258.3127 \\ -13.6398 & -0.0215 \end{pmatrix}$$

$B1$ = [−10.7942 0.5115 91.5124 −8.5609 0.5149]

$W2$ = 1.0e + 004* [0.0011 1.8295 −0.0026 0.0088 −1.8215],

$B2$ = 5.9317.